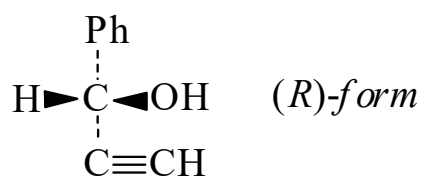




>>Entry Name: 1-Phenyl-2-propyn-1-ol

Synonym(s): α -Ethynylbenzenemethanol, 9Cl. Ethynylphenylcarbinol. 2-Hydroxy-2-phenylpropyne



CAS Registry Number: 4187-87-5

Related CAS Registry Numbers(s): 64937-86-6

Molecular Formula: C₉H₈O

Molecular Weight: 132.162

Accurate Mass: 132.057515

Percentage Composition: C 81.79%; H 6.10%; O 12.11%

Aldrich: 22661-0

Fluka: 78980

Rare Chemicals Library: S46089-3

>>Variant: (R)-form

CAS Registry Number: 61317-73-5

Molecular Formula: C₉H₈O

Molecular Weight: 132.162

Accurate Mass: 132.057515

Percentage Composition: C 81.79%; H 6.10%; O 12.11%

Physical Description: Liq.

Optical Rotation: $[\alpha]_{\text{D}} -27.1$ (c, 2.42 in CHCl₃) (100% op)

Density: d_4^{20} 1.067

Refractive Index: n_{D}^{20} 1.5510

Fluka: 78978

>>Derivative: 2-Carboxy-3-nitrobenzoyl

Melting Point: Mp 152-155°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -53.9$ (c, 2.17 in CHCl₃)

>>Variant: (S)-form

CAS Registry Number: 64599-56-0

Molecular Formula: C₉H₈O

Molecular Weight: 132.162

Accurate Mass: 132.057515

Percentage Composition: C 81.79%; H 6.10%; O 12.11%

Use/Importance: Chiral building block

Physical Description: Liq.

Optical Rotation: $[\alpha]_{\text{D}}^{25} +27$ (c, 1.35 in CHCl₃)

Density: d_4^{20} 1.067

Refractive Index: n_{D}^{20} 1.5510

Fluka: 78976

>>Variant: (±)-form

Molecular Formula: C₉H₈O

Molecular Weight: 132.162

Accurate Mass: 132.057515

Percentage Composition: C 81.79%; H 6.10%; O 12.11%

Physical Description: Prisms

Melting Point: Mp 22°

Boiling Point: Bp₁₂ 114°